Application of Multimedia Models for Screening Assessment of Long-Range Transport Potential and Overall Persistence

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We propose a multimedia model-based methodology to evaluate whether a chemical substance qualifies as POP-like based on overall persistence (P_{ov}) and potential for long-range transport (LRTP). It relies upon screening chemicals against the P_{ov} and LRTP characteristics of selected reference chemicals with well-established environmental fates. Results indicate that chemicals of high and low concern in terms of persistence and long-range transport can be consistently identified by eight contemporary multimedia models using the proposed methodology. Model results for three hypothetical chemicals illustrate that the model-based classification of chemicals according to P_{ov} and LRTP is not always consistent with the single-media half-life approach proposed by the UNEP Stockholm Convention and that the models provide additional insight into the likely long-term hazards associated with chemicals in the environment. We suggest this model-based classification method be adopted as a complement to screening against defined half-life criteria at the initial stages of tiered assessments designed to identify POP-like chemicals and to prioritize further environmental fate studies for new and existing chemicals.

Introduction

The presence of certain organic chemicals in remote areas such as the Arctic has provoked efforts to protect human populations in these regions and the environment from unjustifiable impacts. International conventions and national chemical regulations have identified lists of especially hazardous persistent organic pollutants (POPs), and established global, continental, or national-level restrictions on their use and production (*1*−*4*). Additional regulatory efforts are now aimed at screening chemicals based on cutoff criteria for chemical properties with the goal of identifying chemicals that may pose unacceptable hazards for more rigorous assessments or for setting limits on production and use. The primary goal of such screening assessments is to avoid past mistakes by triggering further studies into the most highly prioritized compounds and ultimately preventing the unrestricted production, use, and release of chemicals that have environmental fate profiles similar to those of well-characterized POPs.

Resistance to degradation and transport over large distances are defining features of the environmental fate of POPs, and screening assessments are therefore designed to identify chemicals that have high environmental persistence and long-range transport potential (LRTP). However, since no direct measurement procedures for environmental persistence and LRTP are available, these assessments must rely on surrogate measures. For example, degradation half-lives have been defined as screening criteria in Annex D of the Stockholm Convention (*1*) for identifying chemicals with potential POP-like behavior. Degradation half-lives of more than 60 days in water or 180 days in soil or sediment, respectively, are used to identify chemicals with high potential to be persistent in the environment, and a half-life of greater than 2 days in air is the screening criterion for atmospheric LRTP.

These degradation half-life criteria represent a simplistic approach to screening chemicals for POP-like behavior in the environment. A more comprehensive assessment requires insight into how substance properties of organic chemicals influence their fate and especially their persistence and long-range transport behavior. Both the scientific and the policy communities have identified multimedia models as valuable tools for providing additional insight in screening assessments of environmental persistence and long-range transport (*5*−*8*). In the Stockholm Convention, for example, it is suggested to use as screening criterion for LRTP "environmental fate properties and/or model results that demonstrate that the chemical has the potential for long-range environmental transport through air, water and migratory species, with the potential for transfer to a receiving environment in locations distant from the sources of release" (*1*).

During recent years, researchers have developed several multimedia models that compute numerical indicators for overall persistence (P_{ov}), which accounts for both degradation half-lives in individual media and environmental partitioning, and a model-specific measure for the long-range transport potential. This paper reports on the results of an expert group convened by the Organization for Economic Cooperation and Development (OECD) to make recommendations for applying multimedia models in the context of screening

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chemicals for POP-like characteristics. In a companion paper, Fenner et al. (*9*) have reported a comprehensive comparison of nine multimedia fate models with respect to the consistency of their P_{ov} and LRTP outcomes. Important differences were identified and characterized, but Fenner et al. concluded that all of the models, if used in their correct context, were appropriate for screening-level assessments of P_{ov} and LRTP for organic chemicals.

In this paper we develop and illustrate a model-based classification methodology for chemicals according to their P_{ov} and LRTP characteristics. The approach is based on cutoff values for high persistence and high LRTP derived from model results for reference chemicals with environmental fate profiles that have been well-characterized by field and laboratory studies as well as monitoring data. We suggest a P_{ov}/LRTP classification plot as introduced by Scheringer (*10*) for visualizing the model results and identifying chemicals with POP-like characteristics. We analyze the consistency of the classification of chemicals among the different models and the effects of parameter uncertainties. Using illustrative examples we demonstrate the additional insight into the environmental behavior of chemicals provided by the proposed model-based screening assessment as compared to the UNEP approach.

Methods

Selection of Reference Chemicals. Our model-based screening method relies upon reference chemicals to which other substances can be compared. The reference chemicals provide a yardstick for assessing the P_{ov} and LRTP of other chemicals. In principle, any chemical with a well-established environmental fate profile could be used as a reference chemical. As a starting point and to illustrate our method, we selected a set of reference chemicals based on (1) extensive experimental evidence of their long-term environmental fate and transport behavior from monitoring data and field and laboratory experiments, and (2) availability of reliable physical−chemical properties and degradation rate constants required by the models. Reference chemicals for high P_{ov} and LRTP have documented evidence in the form of environmental monitoring data and laboratory or field studies that indicate (1) appreciable transport to regions remote from sources, and (2) very slow degradability in the environment. Reference chemicals with well-established low environmental persistence and LRTP were also selected based on a weight-of-evidence approach that considered historical use and release patterns, information on degradability from laboratory studies, and field measurements as well as monitoring data. Using these criteria, we selected 10 reference chemicals that represent a wide spectrum of different long-range transport behaviors and environmental persistence. We used six reference chemicals, for which evidence of POP-like environmental behavior exists, to define model-specific boundaries for P_{ov} and LRTP: three polychlorinated biphenyls PCB-28, PCB-101, and PCB-180, hexachlorobenzene (HCB), α-hexachlorocyclohexane (α-HCH), and tetrachloromethane (CCl_4). Additionally, we included four substances known to exhibit moderate or low LRTP and/or persistence (aldrin, atrazine, biphenyl and *p*-cresol) as reference chemicals to confirm the validity of the boundaries. A detailed discussion of evidence used to support inclusion as a reference chemical is provided in the Supporting Information.

To represent parameter uncertainty and variability, we considered for each reference chemical estimated high, median, and low values of the partition coefficients K_{aw} and K_{ow} and the half-lives in air, water, soil, and sediment. For the partition coefficients we assumed an uncertainty factor of 3 between high and low values. Because degradation rate constants are not only uncertain, but also variable in the environment, we chose a larger variation of a factor of 10 for the half-lives. To restrict the number of possible parameter combinations, we assumed a covariance of 1.0 among the half-lives in the different media. Each reference chemical is therefore represented by $(3^3) = 27$ possible combinations of K_{aw}, K_{ow}, and degradability.

Multimedia Models Used. Eight publicly available multimedia models that are suitable for calculating overall persistence and long-range transport potential were included in the study: ChemRange (*11*), ELPOS (*12*), CalTOX (*13*), SimpleBox (*14*), Impact 2002 (*15*), CEMCLIII (*16*), Globo-POP (*17*), and BETR North America (*18*). Detailed information on model structure and availability can be found in Table 1 in Fenner et al. (*9*) and references therein.

All models except Globo-POP assume steady-state conditions (level III). With the dynamic (level IV) model Globo-POP, simulations of very water soluble substances ($\log K_{aw} < -5$) such as atrazine require extremely small time increments for the numerical solution of the model equations, which made it impossible to include atrazine simulations with Globo-POP in the current study. In contrast to all other models SimpleBox, Globo-POP, and BETR North America consider temperature effects by assigning different temperatures to the different climatic zones or geographical regions, respectively.

Indicators for Overall Persistence and Long-Range Transport Potential. Globo-POP calculates P_{ov} from the ratio of the total mass in the environment to the cumulated reactive mass flux over 10 years of continuous emission. All other models calculate P_{ov} as the reactive residence time in a multimedia environment at steady-state (τ_{ov}) (*19*). For LRTP various different metrics have been proposed which can be separated into transport-oriented and target-oriented metrics. A detailed description of how the models calculate the individual indicators can be found in the Supporting Information of Fenner et al. (*9*).

Transport-oriented metrics are distance-related measures that either estimate the fraction of the total emission (between 0 and 1) carried out of the source region and thus transported over a fixed distance at steady state (SimpleBox and Impact2002) or the distance traveled by a chemical during its lifetime in the environment. ELPOS and CEMC LIII compute the characteristic travel distance (CTD) for complete emission into a single mobile medium (*20*), whereas CalTOX calculates the transport distance (L) for concurrent advective transport in water and air (*21*). ChemRange models dispersive transport between latitudinal zones in a global environment and computes the 95th percentile of the mass distribution of a single, continuous emission either into air, water, or soil as the "spatial range" (R) with possible values between 0 and 0.95 (*22*).

Target-oriented models not only consider long-range transport but also the potential for deposition to surface media in a selected target region. Thus, these models additionally take into account the associated contamination potential in the defined target region. BETR North America uses the ratio of the deposition rate to the Great Lakes and the rate of emissions into the source region to compute the Great Lakes Transport Efficiency (GLTE, %) from a spatially resolved steady-state model of North America. Globo-POP calculates an Arctic Contamination Potential (eACP10, %) as the mass present in the surface media of the Arctic after 10 years of continuous release divided by the total mass emitted into the system over this time period. Emission sources in BETR North America and Globo-POP were selected to be located far away from the target region to allow for an evaluation of long-range transport and subsequent deposition of the chemicals.

The Remote State. All LRTP measures and P_{ov} depend on the emission scenario assumed in the model calculations, i.e., whether emissions are to air, water, or soil. Stroebe et

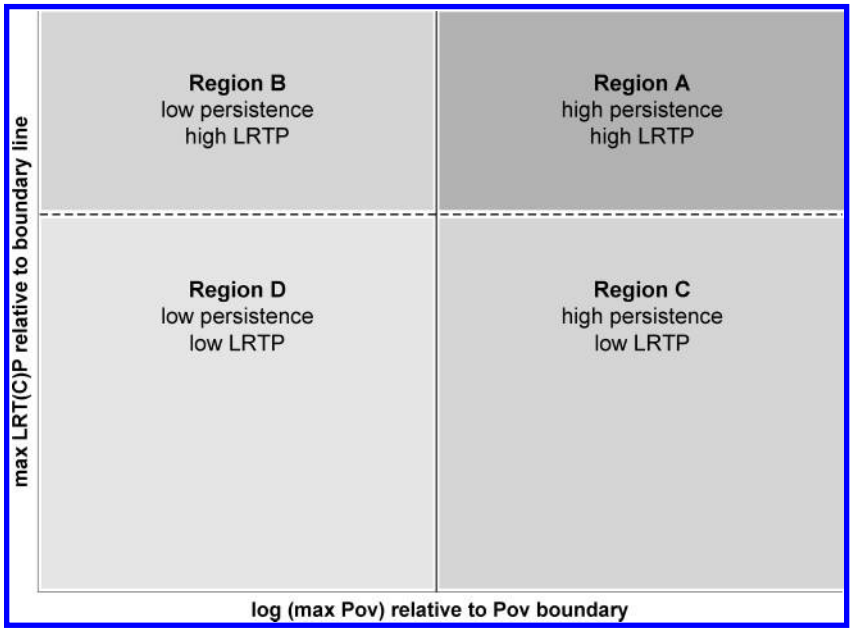

FIGURE 1. Classification of chemicals according to their maximum P_{ov} and LRTP relative to model-specific boundaries.

al. (*23*, *24*) have argued that the most appropriate metrics of P_{ov} and LRTP for hazard assessment are derived from the "remote state" of the chemical−environment system. The spatial and temporal remote states represent the distribution of the chemical in the environment far from sources and long after emissions have ceased. They are independent of emission quantity and mode of entry. An assessment based on the remote state is conservative, since the scales are determined by the most persistent and/or the most mobile fractions of the emitted chemical. A useful surrogate for the remote state is the maximum computed value of P_{ov} and LRTP, respectively, for the various possible single-media emission scenarios. Therefore, for each model, we have calculated P_{ov} and LRTP independently for the single-media emission scenarios (air, water, and soil) and adopted the maximum P_{ov} and LRTP for our assessment.

Classification Approach. Figure 1 shows the generic P_{ov}/LRTP plot that provides the basis for our classification methodology. The maximum values of P_{ov} and LRTP for emissions to air, water, and soil are plotted against each other. Model-specific boundaries are defined by the lowest model outcome of selected reference chemicals with empirical evidence of high persistence and high LRTP (here 3 PCB congeners, HCB, α-HCH, CCl_4). A vertical line forms a boundary between chemicals with high P_{ov} and less persistent substances, and a horizontal line separates chemicals with POP-like potential for long-range transport from those that are expected to be less mobile in the environment. As a result there are four classes of chemicals which are distinguished by their overall persistence and LRTP (Figure 1).

Highest priority is assigned to chemicals that exhibit both POP-like LRTP and P_{ov}. These chemicals are located in the top right corner (region A) of the classification plot. Chemicals situated in the bottom left corner (region D) have non-POP-like P_{ov} and LRTP, and are of lowest priority. Substances in the two other regions (regions B and C) exhibit POP-like characteristics for one indicator and are assigned an intermediate priority.

Results and Discussion

Figures 2 and 3 present classification plots for the transport-oriented models and Figure 4 is the plot for the target-oriented models. The six reference chemicals with empirical evidence for high LRTP and high P_{ov} are shown as triangles, the four others are represented as circles. For each substance, the large symbols represent the model outcome for the default values of the input parameters whereas the smaller symbols indicate model outputs for the other 26 property combinations.

Although the eight models are different in model structure and parametrization, plots of the results are qualitatively similar with respect to the location of the reference chemicals within the P_{ov}/LRTP space, which is in agreement with the findings of the model comparison study of Fenner et al. (*9*). The three PCBs, HCB, and α-HCH are all located in the top right quadrant of the classification plots in all models, consistent with their empirically documented high LRTP and overall persistence. CCl_4 shows very high persistence and LRTP in all transport-oriented models (Figures 2 and 3). This is consistent with its known behavior in the environment, where it has been demonstrated to be persistent and mobile in the atmosphere. However, since CCl_4 is not efficiently deposited to surface media in remote areas it exhibits a relatively lower LRTP in the two target-oriented models (Figure 4) compared to the transport-oriented ones.

All plots include a line of maximum LRTP in the atmosphere for a given P_{ov}. For transport-oriented indicators this "*volatility line*" represents a physical limit on transport potential in the atmosphere defined by a hypothetical substance that partitions entirely into air. This line is straight when CTD is the LRTP metric (Figure 2), but it takes on an S-shape for bounded indicators such as those used in ChemRange, IMPACT2002, and SimpleBox (Figure 3). When only transport in the atmosphere is considered, no substances will be found above the volatility line because it represents the maximum possible mobility in the atmosphere for a given overall persistence. However, some models account for simultaneous transport in the atmosphere and surface or ocean waters. In these models it is possible for substances to have greater LRTP than a volatile chemical with the same overall persistence. This is the case for ChemRange, for example, where HCB and CCl_4 are located slightly above the volatility line (Figure 3). In target-oriented models volatile chemicals do not define an upper limit on LRTP since this metric additionally considers deposition from the atmosphere to a target water body or region. Maximum lines for BETR North America and Globo-POP have thus been empirically estimated from simulation results obtained for a compre-

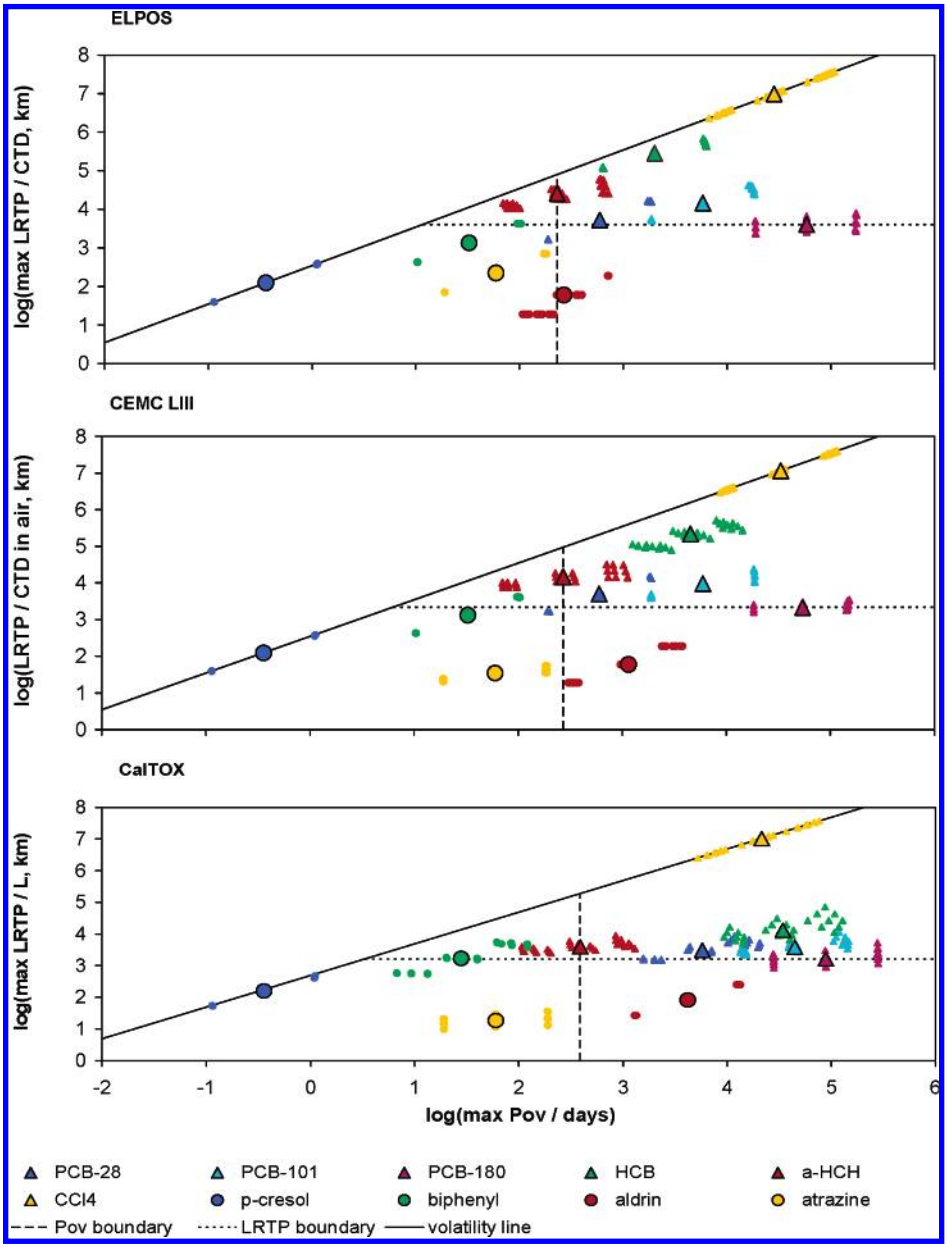

FIGURE 2. LRTP/P_{ov} classification plots for selected reference chemicals with transport-oriented models using distance metrics for LRTP.

hensive set of hypothetical chemicals used in the model comparison study by Fenner et al. (*9*).

Classification Boundaries. Model-specific boundaries for P_{ov} and LRTP were derived from the model results as the minimum values of the six selected high P_{ov}/high LRTP reference chemicals based on the geometric means of the substance properties. The persistence boundary is determined by α-HCH except with IMPACT2002, where PCB-28 exhibits slightly lower values. The P_{ov} boundary values are similar for six of the models (176−359 d), with SimpleBox (512 d) and Globo-POP (1259 d) exhibiting higher values. Because SimpleBox assumes an average temperature of 12 °C with an automatic correction of the degradation rate constants, one obtains higher numerical values of P_{ov} with this model. The significantly larger P_{ov} values calculated by Globo-POP can be similarly explained by the adjustment of the degradation rate constants to seasonally and zonally variable temperatures.

On the LRTP scale, boundaries are defined either by CCl_4 (BETR North America), PCB-28 (Globo-POP, ChemRange), or PCB-180 (all other models) with maximum LRTP always for the air-release scenario. The LRTP of the highly persistent PCB-180 is mainly limited by deposition from the atmosphere of the particle-bound fraction, whereas for PCB-28 degradation in air is the process limiting long-range transport. ChemRange and Globo-POP assume a larger volume air compartment than the other models. As a result they give higher weight to the atmospheric degradation process than to particle deposition (*25*). This explains the smaller LRTP values of PCB-28 provided by ChemRange and Globo-POP.

The four reference chemicals that do not meet both criteria—*p*-cresol, biphenyl, aldrin, and atrazine—are consistently classified by all models with low values of LRTP and/or P_{ov}. For biphenyl low P_{ov} values below the persistence boundary are calculated, but LRTP values are close to the boundary. In CalTOX biphenyl receives an LRTP just above the boundary value (Figure 2), which is attributable to differences in compartment dimensions and process rate constants that affect steady-state mass partitioning (*9*). In accordance with the long half-lives in water (111 days) and sediment (1114 days), aldrin exhibits relatively high P_{ov} values with the maximum for the water emission scenario. Although

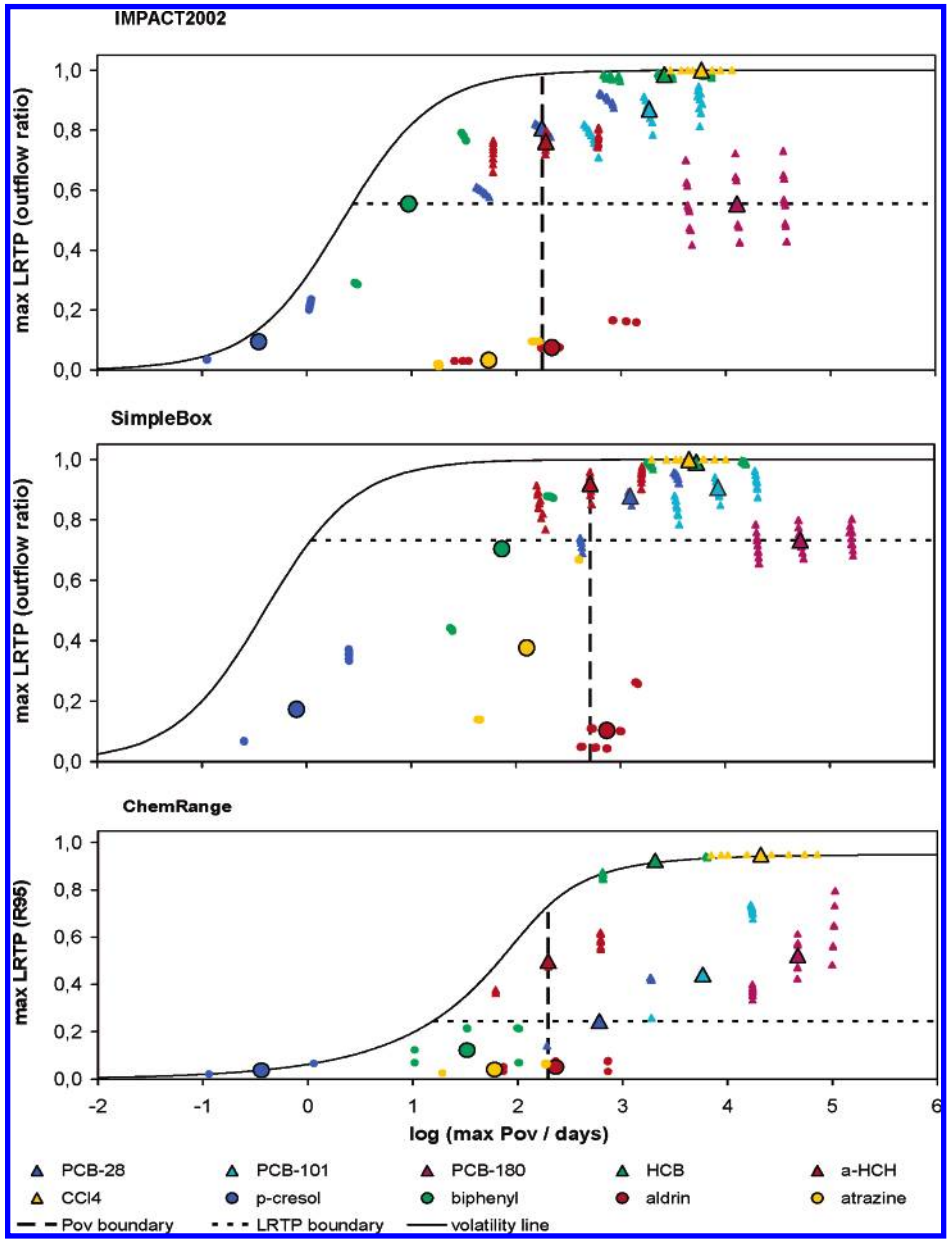

FIGURE 3. LRTP/P_{ov} classification plots for selected reference chemicals with transport-oriented models using percentage metrics for LRTP.

aldrin is identified as a POP in the Stockholm Convention, its short atmospheric half-life results in a low atmospheric LRTP. Since the compound is trapped in the sediment due to its high K_{ow}, LRTP in water is also small. Aldrin is consequently classified as having high persistence but a low LRTP (region C) in all models. Atrazine has a strong tendency to partition to water and in some models exhibits higher LRTP values for transport in water than in air, but still lies clearly below the LRTP boundary. On the P_{ov} scale it is located below the boundary in all models, although it exceeds the UNEP half-life criterion for persistence in sediment (421 days). It is classified as nonpersistent with low LRTP (region D) by all models.

Influence of Parameter Uncertainty. Uncertainty and variability of substance parameters affect calculated P_{ov} and LRTP values. This is illustrated by the 27 data points generated for each reference chemical by assuming upper and lower bounds of half-lives and partition coefficients (Figures 2−4). The simultaneous change of all half-lives causes an almost linear change in P_{ov} and LRTP of all reference compounds with data points approximately covering the range of uncertainty attributed to the half-lives (factor of 10). Variation of the partition coefficients mainly affects the LRTP values. Since the uncertainty assumed for the partition coefficients is smaller (factor of 3), the observed scatter of data points in this case is also smaller than for the variation of half-lives. Some model results are even completely insensitive to the change of partition coefficients within the prescribed range. In those cases the 27 data points are not all resolved in the plots, e.g., for *p*-cresol all property combinations representing a specific degradation half-life combination overlap (Figure 2−4).

In terms of applying the P_{ov}/LRTP classification plots to screen chemicals, there are two important implications of this uncertainty analysis. First of all, the classification depends on the selection of appropriate reference chemicals. A different set of reference chemicals with similar properties would lead to somewhat different boundary lines. Thus, the boundaries shown here should be viewed only as approximate guidelines and not as the ultimate separating lines when interpreting results. Second, model results—including those used to define the boundaries and those for placing chemicals

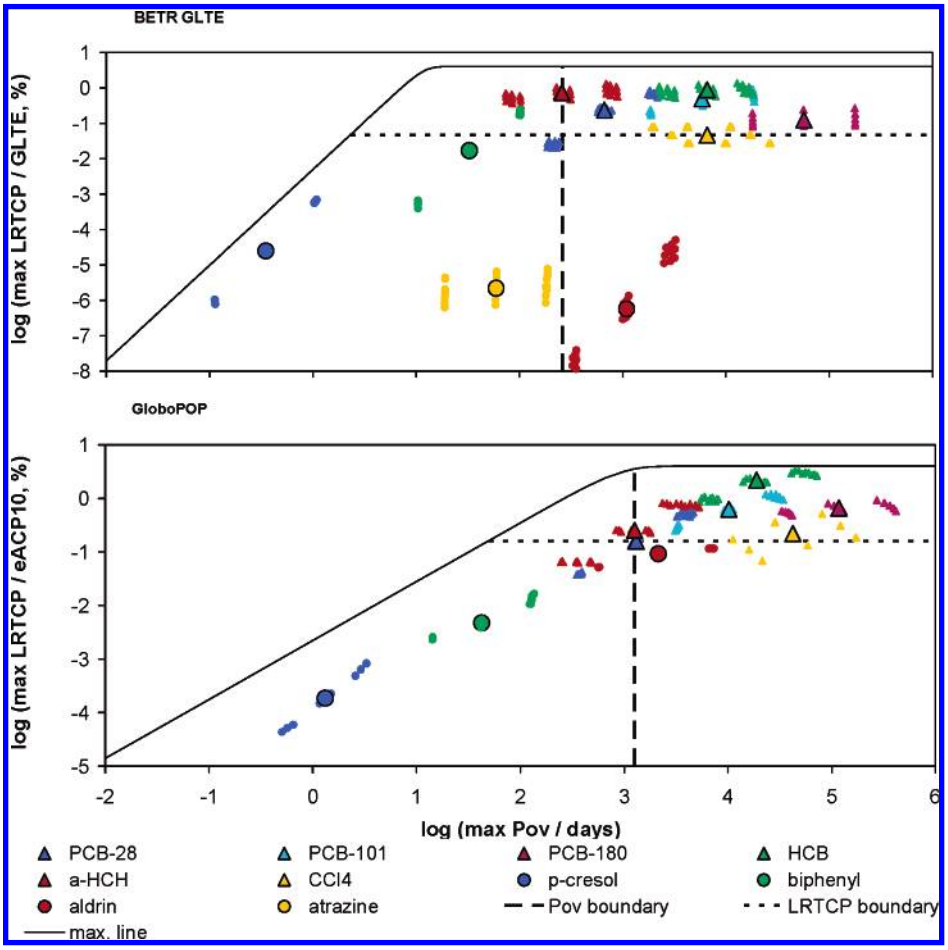

FIGURE 4. LRTP/P_{ov} classification plots for selected reference chemicals with target-oriented models.

TABLE 1. Important Substance Properties of Hypothetical Chemicals Used for Illustration of the Model-Based Classification Methodology (Bold Values Indicate Exceedance of UNEP Criterion)

substance label	log K_{ow}	log K_{aw}	HL_{air}[a] (days)	HL_{water}[a] (days	HL_{soil}[a] (days	$HL_{sediment}$[a] (days	Classification	UNEP	model-based
Hypo-A	5.0	−4.0	**7**	41.7	83.3	**417**	P[b]	yes	no
							LRTP	yes	no
Hypo-B	5.0	2.0	**365**	7	14	70	P[b]	no	yes
							LRTP	yes	yes
Hypo-C	0.0	−5.0	0.17	**3650**	**7300**	**36 500**	P[b]	yes	yes
							LRTP	no	no[c]/yes[d]
UNEP criterion			>2	>60	>180	>180			

[a] HL = half-life. [b] P = persistence. [c] For transport in air. [d] If transport in water is considered.

within these boundaries—should not be interpreted without recognizing that uncertainty in input parameters propagates through the calculations. Classification of chemicals with this model-based approach is only as reliable as the input data for the reference and the target chemicals.

Illustrating Examples. The utility of the proposed model-based classification method can best be illustrated using hypothetical example chemicals (Table 1) near the boundaries of the single half-life categorization criteria proposed in Annex D of the Stockholm Convention. In Figure 5 results from the eight models for the three chemicals specified in Table 1 are schematically displayed to represent their location in the P_{ov}/LRTP space relative to the different boundary values of the individual models. Compound Hypo-A exceeds the UNEP single-media half-life criteria for both persistence and LRTP. However, results from the model-based approach suggest a different classification. Because of its low K_{aw} and high K_{ow} values Hypo-A partitions only marginally into air resulting in a non-POP-like LRTP (below the boundary). This model-based interpretation could be used in conjunction with the provisions of Annex D of the Stockholm Convention where the 2 days half-life criterion in air is defined as a cutoff criterion "... for a chemical that migrates significantly through the air, ...". Additionally, all models but one (CalTOX) compute P_{ov} values below the boundary indicating that single media persistence (e.g., in sediment) does not necessarily imply high overall persistence.

For Hypo-B, which is volatile and resistant to degradation in the atmosphere, transport-oriented models calculate POP-like P_{ov} and LRTP, both above the boundary (region A). The target-oriented models additionally consider deposition in the target region, which is not efficient for this volatile chemical resulting in a non-POP-like classification according to their LRTP. In other words, highly volatile chemicals that

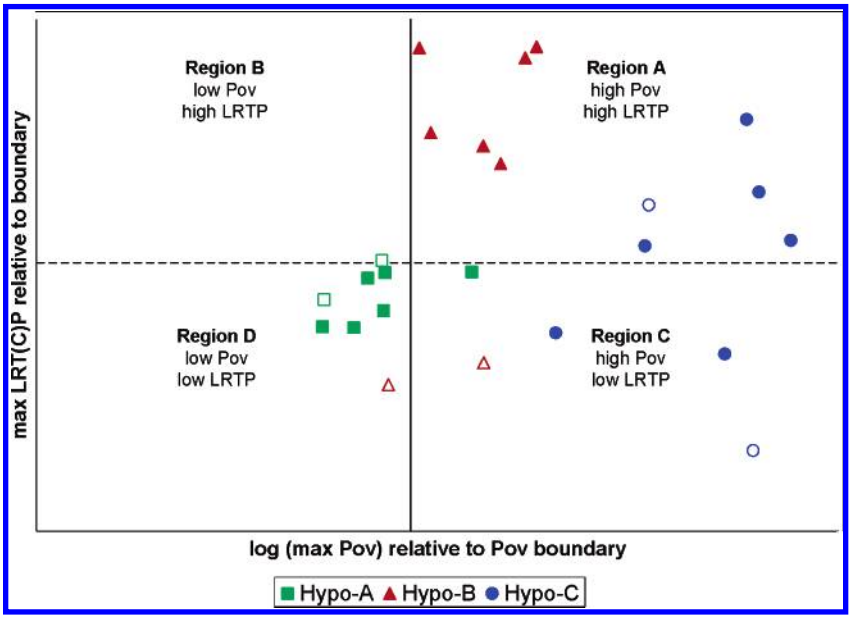

FIGURE 5. Location of three hypothetical chemicals in the P_{ov}/LRTP classification plot relative to the model-specific boundaries. Full symbols represent results from transport-oriented models, open symbols represent results from target-oriented models; all values have been scaled to represent the relative location to the respective model-specific boundary.

are persistent in air are POP-like chemicals in terms of LRTP and persistence, but do not necessarily meet the additional criterion of "... transfer to a receiving environment in locations distant from the sources of its release." given in Annex D (3d (iii)) of the Stockholm Convention. This is further illustrated by the results obtained for the reference chemical CCl_4 and demonstrates the effect of considering deposition processes as measures of impact in the target-oriented models. The choice of whether to consider the additional deposition criterion as done in the target-orientated approaches will depend on the decision-making context. This example shows that the application of different models delivers additional information, which can be used for a more detailed assessment.

Results for Hypo-C highlight the effect of waterborne transport mentioned as LRTP criterion in Annex D (1d (iii)) of the Stockholm Convention on the assessment of chemicals. Hypo-C represents a hydrophilic chemical (very low K_{aw} and K_{ow}) with a short half-life in air, but long half-lives in water, soil, and sediment. On the P_{ov} scale all models agree with the UNEP criteria classifying this substance as having POP-like persistence. However, the five models that give a relatively high weight to transport in water (ELPOS, SimpleBox, ChemRange, IMPACT2002, and Globo-POP) also indicate high LRTP, which cannot be accounted for by the single half-life in air criterion. Since CEMC LIII and BETR North America do not consider transport in water and CalTOX uses a continental environmental parametrization with very little water, maximum LRTP in these models is given by the air scenario and is consequently low. In other words, for hydrophilic substances transport in water may be more important than transport in air, so that the half-life in air is inadequate as the sole criterion to assess LRTP. The maximum LRTP approach proposed here can close this gap by considering the potential for transport in water. The eight multimedia models, however, differ significantly with respect to how they treat transport in air and water and thus deliver different interpretations, which can provide important insight in a decision-making context.

These examples illustrate the additional information that is available from the proposed model-based methodology for screening-level assessment and prioritization of chemicals. The approach can yield classifications qualitatively different from those based on the existing UNEP criteria. We suggest that screening criteria based on half-life cutoff values should be supported by the additional insights provided by multimedia models. Different models deliver different information, which in part is dependent on the model structure and the processes included (e.g., additional deposition criterion in target-oriented model and emphasis on transport in water) and can be considered in the decision-making process. Multimedia models thus facilitate screening and assessment of chemicals for POP-like characteristics in a way that is not possible with single-property classification schemes. We recommend that the model-based P_{ov}/LRTP assessment be incorporated into the process for identifying chemical substances that pose unacceptable environmental hazards due to their inherent properties as described in the Stockholm Convention.

Acknowledgments

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Supporting Information Available

Empirical evidence of persistence and long-range transport, physico−chemical substance properties and degradation half-lives for ten reference chemicals, and references. This material is available free of charge via the Internet at http://pubs.acs.org.

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